

PROJECT NUMBER: 1754
PROJECT TITLE: Spectroscopic Studies of Tobacco and Smoke Components
PROJECT LEADER: J. B. Wooten
PERIOD COVERED: April, 1988

I. SOLUTION NMR OF TOBACCO COMPONENTS

- A. Objective: Determine the composition and structure of tobacco cell wall biopolymers (J. Wooten, S. Baldwin).
- B. Results: The ^{13}C NMR spectrum of tobacco hemicellulose was obtained and the results were correlated with the neutral sugar analysis. The sample was found to contain 40% glucose, 17% galactose, 16% xylose with smaller amounts of other sugars. Not surprisingly, the NMR spectrum of such a complex material is complicated, but numerous distinct spectral features were observed including 7 resolved anomeric carbon resonances. Of particular note was the absence of any signal at 103.2 ppm. The anomeric carbon signal of glucose having two contiguous glucose residues appears at 103.2 ppm. This indicates that the hemicellulose does not contain significant Glu-Glu-Glu units (or larger Glu groups) and that the glucose is distributed randomly with the remaining sugars. The analysis of this material is continuing.
- A. Objective: NMR analysis of 2-cyclohexene-1-one derivatives (R. Bassfield, K. Podraza).
- B. Results: The complete spectral assignments of the ^1H and ^{13}C NMR spectra of five cyclohexenone derivatives were made using one and two dimensional NMR techniques. The ^1H - ^1H coupling constants were used to define the orientation of the alkyl substituents on the cyclohexenone ring.

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